



chain nodes :  
 15 16 19 20 21 22

ring nodes :  
 1 2 3 4 5 6 7 8 9 10 11 12 13 14

chain bonds :  
 2-19 7-15 10-16 12-20 19-22 20-21

ring bonds :  
 1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-10 7-8 8-9 8-11 9-10 9-14 11-12 12-13 13-14  
 exact/norm bonds :  
 1-2 1-6 2-3 2-19 3-4 4-5 5-6 5-7 6-10 7-8 7-15 8-9 8-11 9-10 9-14 10-16 11-12  
 12-13 12-20 13-14 19-22 20-21

G1:Cl,Br,F,I,CH3,Et,n-Pr,s-Bu,CF2,CN,C,S,N,Si,H

G2:C,N

G3:C,H,S,N,I

Match level :  
 1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom  
 12:Atom 13:Atom 14:Atom 15:CLASS 16:CLASS 19:CLASS 20:CLASS 21:CLASS 22:CLASS